Pentafluoropropionic acid 422-64-0 | DTXSID8059970

Model Performance

Model	Data	

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 100 °C

Global applicability domain: Inside

Local applicability domain index: 4.94e-01

Confidence level: 6.40e-01

Nearest Neighbors from the Training Set

Image not found

Pentafluoropropionic acid

Measured: 96.5 Predicted: 100

Image not found

Heptafluorobutyric acid

Measured: 121 Predicted: 120

Image not found

Flupropanate

Measured: 134 Predicted: 126

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Acetic acid, trifluoro-Measured: 73.0 Predicted: 85.2

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Acetic acid, chlorodifluoro-

Measured: 122 Predicted: 128